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A SENSITIVITY ANALYSIS FOR DETERMINING OPTIMUM WRF AND CALPUFF CONFIGURATION FOR OPERATIONAL AIR QUALITY FORECAST: APPLICATION TO A CASE STUDY IN THE PORT OF HUELVA (SOUTHERN SPAIN)

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Abstract: Meteorological inputs are of great importance when implementing an air quality modelling system. The aim of this study is to define a standardized methodology to determine the best meteorological configuration to reduce the uncertainty of the model predictions. To do this, a detailed sensitivity analysis to different parameterizations and schemes of the Weather Research and Forecast (WRF-ARW) model has been realized. The sensitivity of the model to different options: physical and dynamical configurations, different vertical levels distribution, and the impact of the high resolution topography and land use data have been evaluated. A sensitive analysis was done in order to evaluate some simulated meteorological variables (temperature, relative humidity, wind velocity and wind direction) and achieve the optimum WRF configuration. Since the better options for WRF simulations were chosen, a new sensitivity analysis was done to determine the optimum CALPUFF-CALMET configuration for air quality forecasting. Changes in number of vertical levels and physical options were done in this analysis.

The study has been realized in a coastal region of Andalusia, in the South of Spain. A period of 4 months for different climatic seasons was used to calibrate adequately the WRF model. Moreover, 2-year period (2012 and 2013) with the optimum configuration from the previous calibration was validated. Numerical deterministic comparison between observed and modelled data has been the methodology analysis used.

Results show a moderate improvement of meteorological predictions when comparing meteorological forecasts using default WRF model options and forecasts using the optimum WRF model configuration over the region of interest. The same is shown for CALPUFF sensitive analysis, where parameters such wind direction achieved better results when optimum CALMET configuration was selected.

Key words: *WRF, CALPUFF, CALMET, Sensitive Analysis, Meteorological Modelling, Air Quality Modelling, Physical options, High Resolution*

INTRODUCTION

The goal of this paper is to achieve the optimum configuration of meteorological model WRF and dispersion model CALPUFF in order to obtain better results in air quality forecasts (Warner, 2011; Stensrud, 2007; Reboredo et al., 2015). A region in Southern Spain, Huelva, was selected for the development of this work. Industrial and port activities, especially aggregate handling and storage piles, are responsible of major of atmospheric pollution existing in this area. An operating prediction system will be used as early warning system and will allow improving the air pollution and risk management associated to the Port of Huelva. The methodology used for sensitive analysis and configurations here defined can be extrapolated to other interesting regions. Meteorological forecasting system developed increases the resolution and the accuracy, not only for meteorological results, but also for air quality and risk management in the zone.

METHODOLOGY

The Port of Huelva is one of the most important industrial sources in the South of Spain. Moreover, this area coexists with the city of Huelva, greenhouse zones and some nature reserves like Doñana Park. Meteorology can greatly affect the atmospheric pollution generated by the Port, because the activities here carried out (loading and unloading operations and material handling) are mainly an important source of particles; meteorological parameters, such as wind speed and wind direction, are highly significant in dispersion of these particles. In this sense, the meteorology influence the atmospheric pollution generated by port activities, in it-self, is conditioned by the meteorological conditions.

Meteorological model

Air quality levels achieved and the risk management in a complex harbour located very near of metropolitan and protected nature areas made important the implementation of a very accuracy meteorological model in the zone. Also, better results in meteorological modelling will lead more accurate results in air quality modelling. Here is defined the methodology to obtain the optimum WRF configuration, and then it was applied over the Port of Huelva and surroundings.

In Figure 1 modeling domains used in simulations are shown. The WRF model is built over a mother domain (called d01) with 9 km spatial resolution, with three nested domains: d02, with a spatial resolution of 3 km, d03, with 1 km of spatial resolution covering Huelva, and d04, with a spatial resolution of 0.333 km covering the Port of Huelva.

d01, d02, d03 and d04 **d04**

Figure 1. Modeling domains for simulations. [Images generated using Google Earth]

Simulations were executed for 30 hours in different periods between 01/01/2012 and 12/31/2013, taking the first 6 hours as spin-up time to minimize the effects of initial conditions. The regional and mesoscale meteorological model used for the study has been the Weather Research and Forecasting - Advanced Research (WRF-ARW) version 3.7 (Skamarock et al., 2008), developed by the National Center of Atmospheric Research (NCAR). The initial and boundary conditions for the operational configuration over domain d01 were supplied by the National Centers for Environmental Prediction (NCEP). For model configuration, calibration and validation, two-way nesting was used for the external domains (d00, d01, d02 and d03) and one-way nesting for d04 innermost domain. Also, in d04 Large-Eddy-Simulation (LES) technique has been applied, which is considered relevant when the horizontal resolution meteorological model works is below 500 m (Dudhia and Wang, 2015).

18 experiments modifying physical options (compared with WRF default configuration), 4 experiments modifying dynamical options, 2 experiments modifying the number and density of vertical levels, 2 experiments modifying land use and topography databases, and 5 experiments applying grid and observational nudging. A sensitivity analysis was done considering the full set of experiments, modifying only one configuration option each time, and holding all else constant. This analysis is going to be the best way to know the optimum configuration for modelling.

Air quality dispersion model

As said before, the coastal region of Huelva is characterized by atmospheric pollution generated as consequence of industrial and port activities among others. Meteorological fields calculated before can be used for air quality and risk management. For this purpose, CALPUFF model was considered; CALPUFF (Scire et al., 2000) is an advanced, integrated gaussian puff modeling system, developed by Atmospheric Studies Group (ASG) and recommended by the United States Environmental Protection Agency (EPA) for atmospheric pollution dispersion studies. This model is appropriated for areas with complex topography and coastal zones like the Port of Huelva.

Domain used in CALPUFF simulation was designed similar to d04 WRF domain, covering the Port of Huelva and surroundings. Horizontal resolution was set in 100 m, in order to achieve reproduce the complex terrain of this area. WRF meteorological fields were adapted by CALWRF model, and then processed by CALMET, taking into account topography information and land use cover. 10 experiments were developed for identifying the better CALMET configuration: changes in number of vertical levels and physical options, such kinematic effects, the O'Brien vertical velocity adjustment, or the diagnostic wind module. Better configuration for the model was selected according to best statistics (Mean Bias, MB, Mean Absolute Gross Error, MAGE, Root-Mean-Square Error, RMSE, and the Index of Agreement, IOA), calculated for each experiment.

Apart from meteorological information, CALPUFF model needs emissions inputs, provided by AEMM (Air Emission Model of Meteosim, Arasa et al., 2013; 2016). Emissions are calculated by the model after taking information of the Integration Platform Operations Authority of Port of Huelva. This platform includes data about emission types, emission sources and their physical characteristics, handled materials stored, and emission process times. With this information and specific emission factors for different materials, AEMM gives emission predictions for TSP, PM_{10} and $PM_{2.5}$. Simultaneously, emissions are also estimated considering some mitigation measures: water sprays, cleaning programmes, or aestivation good practices. The last step, postprocessing, is done with CALPOST module. Analysis of dispersion results and statistics are calculated by CALPOST with the purpose of compare with legislated values.

RESULTS

A sensitive analysis was done in order to determine the optimum configuration for WRF model. Physical options, dynamical options and physiographic databases were manipulated and tested. Some meteorological parameters were modelled and compared with observed values, specifically temperature, wind speed, wind direction and relative humidity in high resolution domains (d03 and d04). Results obtained by the whole group of experiments were compared individually with an experiment done with WRF default configuration. A local meteorological station inside the Port of Huelva (37.20ºN, 6.93ºW) was incorporated to compare the performance obtained in these high resolution domains. A statistical evaluation (Denby et al., 2008) was done for each experiment; metrics have been calculated from hourly data of the model and observations. For summarize the sensitive analysis, in Table 1 are shown all the selected options for that configuration whose statistical evaluation was the best. This configuration showed the best results for temperature, wind speed, wind direction and relative humidity predictions.

Table 1. Configuration options selected as optimum for meteorological forecast over the coastal region of Huelva

Scheme or parameterization	Selected option
Initialization	GFS 0.25º
Microphysics	SBU-Lin
Longwave radiaion	RRTMG
Shortwave radiation	Dudhia
Cumulus	Kain-Fritsch
Surface Layer	MM5 similarity
Planetary Boundary Layer	YSU (9, 3 and 1 km) / LES (0,333 km)
Vertical levels number	36
Diffusion 6th order option	Knievel
Diffusion 6th order factor	0.36 (d03)
Damping	Rayleigh
Topography	GTOPO30 (9 and 3 km) / ASTER (1 and 0,333 km)
Land Uses	GLC (9 and 3 km) / CLC2006 (1 and 0,333 km)
Nudging	Grid nudging (9 km) / Observational nudging (3 and 1 km)

Statistical evaluation is also was done for air quality forecast, taking into account some meteorological parameters, by comparing the modelled parameters to the meteorological station observations of temperature at 2 m, wind speed at 10 m, wind direction at 10 m and relative humidity at 2 m. Options that provided better results, and therefore, were selected, are listed in Table 2; also, metrics obtained for this configuration are shown and compared with benchmarks (Emery and Tai, 2001; Tesche et al., 2002; Arasa et al., 2012) in Table 3. Slight improvement was achieved in wind speed RMSE, and also in wind direction better metrics were obtained, with MB values from 3.73° to 3.20° and MAGE values from 20.18° to 18.86°.

Table 2. Configuration options selected as optimum for meteorological forecast over the coastal region of Huelva

Scheme or parameterization	Selected option
Kinematics effects	IKINE Activated
O'Brien vertical velocity adjustment	IOBR Activated
Diagnostic wind module	IWFCOD Activated
Vertical levels number	20
Topography	ASTER 1s
Land Uses	CLC2006 100m

Table 3. Comparison between modelled and observed values in CALPUFF calibration experiments

Meteorological parameter (reference height)	Statistic	Benchmark	Statistic values for optimum WRF configuration and CALMET default configuration	Statistic values for optimum WRF configuration and CALMET optimum configuration
Temperature (2 m)	MB	< ±0.50 K	0.58	0.58
	MAGE	< 2.00 K	1.19	1.19
	IOA	≥ 0.80	0.98	0.98
Wind speed (10 m)	MB	±0.50 ms^{-1}	-1.64	-1.64
	RMSE	< 2.00 ms^{-1}	2.26	**2.13**
Wind direction (10 m)	MB	< ±10.00°	3.73	**3.20**
	MAGE	< 30.00°	20.18	**18.86**
Relative humidity (2 m)	MB	< 10.00%	0.89	0.89
	MAGE	< 20.00%	6.29	6.29
	IOA	≥ 0.60	0.93	0.93

An operating prediction system was developed for the Port of Huelva. Meteorological and air quality forecasting had been integrated in a platform which allows visualize all the predictions. Prediction system is actualized four times a day, and various types of air quality forecasting are shown. First, dispersion of each pollutant is calculated without considering mitigation measures in emission estimation. Then, three different mitigation measures (cited above) are added, and therefore three new air quality forecasting are obtained for each pollutant (one with each mitigation measure). This methodology lets the user to compare and to know the differences between different air quality predictions, when mitigation measures in industrial and port activities are considered or not.

Apart from hourly meteorological variables and fields, multiple maps and tables for atmospheric pollution are included in operating prediction system, and they are actualized each six hours in order to obtain the highest accuracy in air quality forecasting. Daily statistics maps for each prediction and pollutant (TSP, PM_{10} and $PM_{2.5}$), time series of selected points of interest near the Port of Huelva, windroses and trajectories calculated with HYSPLIT model (Stein et al., 2015) are displayed. As an example, Figure 2 shows some maps for air quality predictions, calculated with CALPUFF model with 100 metres of horizontal resolution, with and without consider mitigation measures.

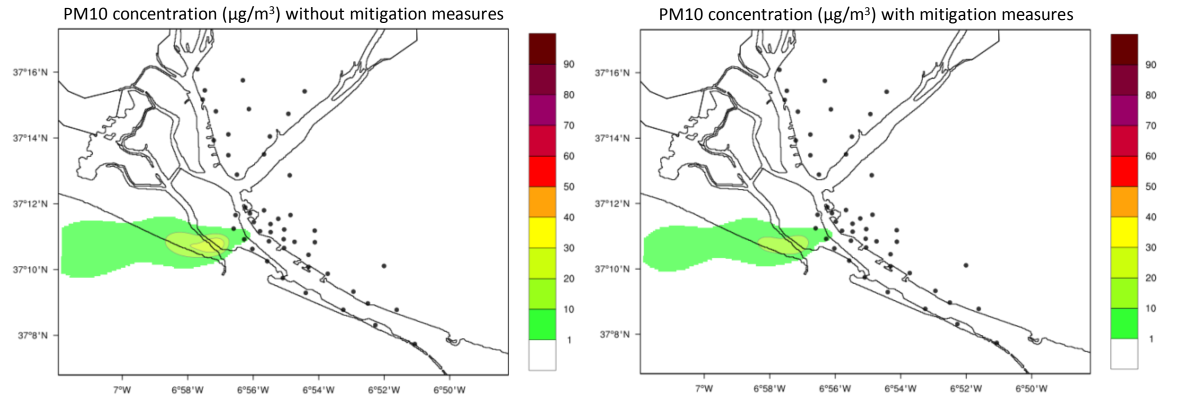

Figure 2. Some examples for air quality forecasting for PM_{10}.

CONCLUSIONS

To improve air quality and to manage more efficiently the daily activity of the Port of Huelva, an air quality modelling system has been developed. A standard methodology to select the optimum meteorological and air quality configuration in any region has been defined. Some experiments modifying parameters such physical options, dynamical options, number of vertical levels, or land use and topography databases were carried out. First, a sensitivity analysis was done for WRF model with the purpose of obtain its optimum configuration; then, a similar methodology was developed for CALPUFF model. Both analyses were useful for determining the best options for modelling air quality in the Port of Huelva. Anyway, this meteorological and air quality prediction system could be developed in any complex region of interest.

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